



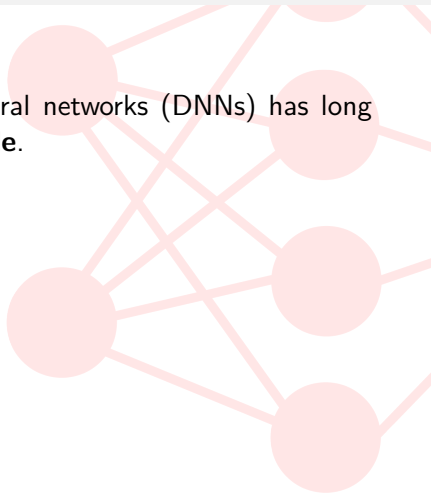
Explainable Network Growth by Folding on Typical Mis-predictions

Jimmy KANG

March 13, 2025

Problem Statement

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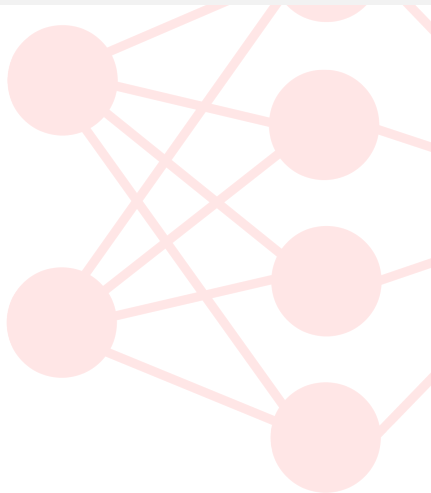
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- The training of artificial deep neural networks (DNNs) has long suffered from their **enormous scale**.
- The black box nature of the training process weakens the **interpretability** of neural network models in understanding of the mechanisms behind their decision-making.
- The existing training strategy initializes **over-parameterized** models and allows representations to be learned in an anarchic manner from large amounts of data.
 - found to **underutilize the approximability** of the model
 - **decision criteria** are arranged in an unordered and susceptible manner

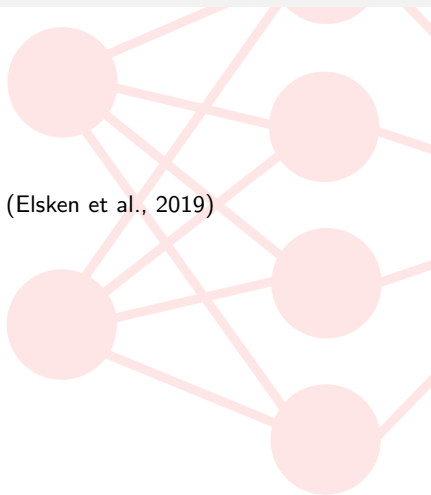
Related works

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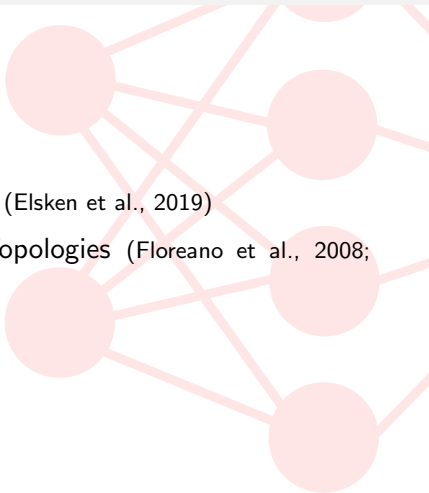
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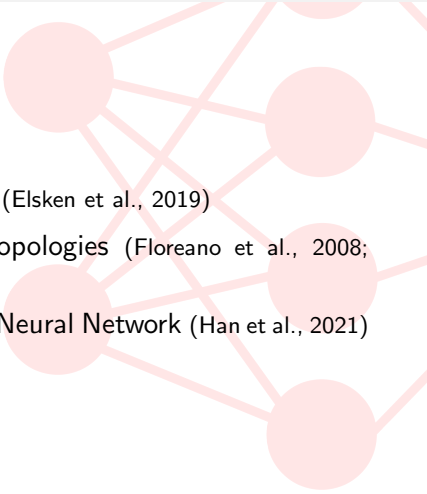


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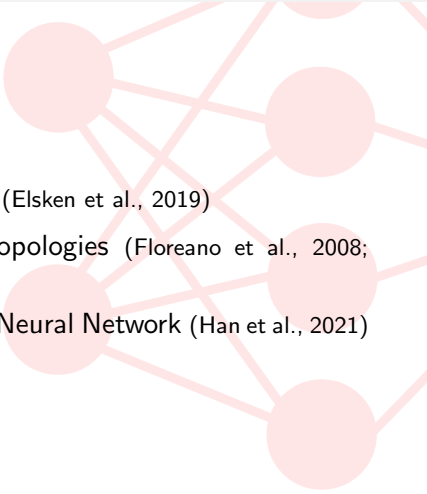
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Published as a conference paper at ICLR 2022

GRADMAX: GROWING NEURAL NETWORKS USING GRADIENT INFORMATION

Utku Evci, Bart van Merriënboer, Thomas Unterthiner,
Max Vladymyrov, Fabian Pedregosa
Google Research, Brain Team
{evcu, bartvm, unterthiner, mxv, pedregosa}@google.com

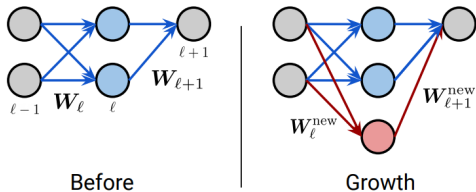
ABSTRACT

The architecture and the parameters of neural networks are often optimized independently, which requires costly retraining of the parameters whenever the architecture is modified. In this work we instead focus on growing the architecture without requiring costly retraining. We present a method that adds new neurons during training without impacting what is already learned, while improving the training dynamics. We achieve the latter by maximizing the gradients of the new weights and efficiently find the optimal initialization by means of the singular value decomposition (SVD). We call this technique Gradient Maximizing Growth (GradMax) and demonstrate its effectiveness in variety of vision tasks and architectures¹.

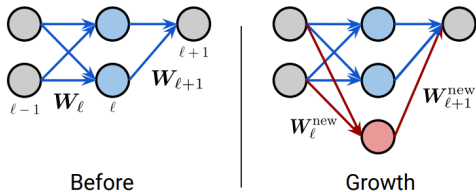
1 INTRODUCTION

The architecture of deep learning models influences a model's inductive biases and has been shown to have a crucial effect on both the training speed and generalization (d'Áscoli et al., 2019; Neyshabur, 2020). Searching for the best architecture for a given task is an active research area with diverse approaches, including neural architecture search (NAS) (Elsken et al., 2019), pruning (Liu et al., 2018), and evolutionary algorithms (Stanley & Miikkulainen, 2002). Most of these approaches are costly, as they require large search spaces or large architectures to start with. In this

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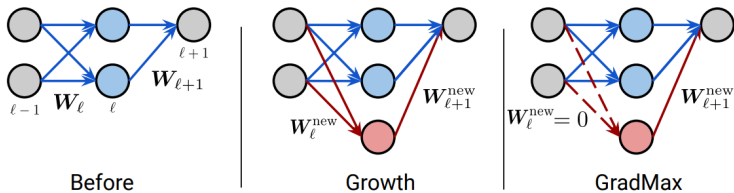
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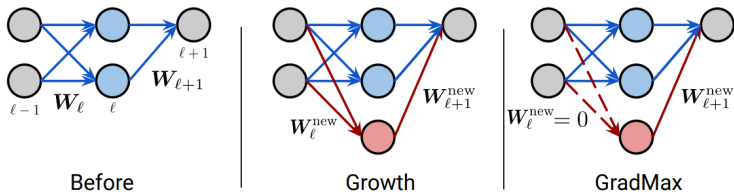
$$W_{\ell}^{+} = \begin{bmatrix} W_{\ell} \\ W_{\ell}^{\text{new}} \end{bmatrix}$$

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$$\arg \max_{\mathbf{W}_{\ell+1}^{\text{new}}} \left\| \mathbf{W}_{\ell+1}^{\text{new}, \top} \mathbb{E}_D \left[\frac{\partial L}{\partial \mathbf{z}_{\ell+1}} \mathbf{h}_{\ell-1}^\top \right] \right\|_F^2, \quad \text{s.t.} \quad \|\mathbf{W}_{\ell+1}^{\text{new}}\|_F \leq c.$$

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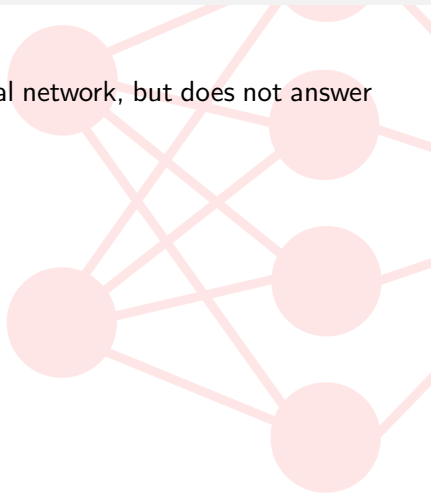
Growing neural networks: When, where and how? Algorithms for growing neural networks start training with a smaller *seed architecture*. Then over the course of the training new neurons are added to the seed architecture, either increasing the width of the existing layers or creating new layers. Algorithms for growing neural networks should address the following questions:

1. **When** to add new neurons? For instance, some methods (Liu et al., 2019; Kilcher et al., 2019) require the training loss to plateau before growing, whereas others grow using a predefined schedule.
2. **Where** to add new capacity? We can add new neurons to the existing layers or create new layers among the existing ones.
3. **How** to initialize the new capacity?

In this work we mainly focus on the question of **how** and introduce a new initialization method for the new neurons. Our approach can also be used to guide when and where to grow new neurons. However, in order to make our comparison with other initialization methods fair we keep the growing schedule (**where** and **when**) fixed.

Baseline: GradMax (Evci, et al., 2022) - Limitations

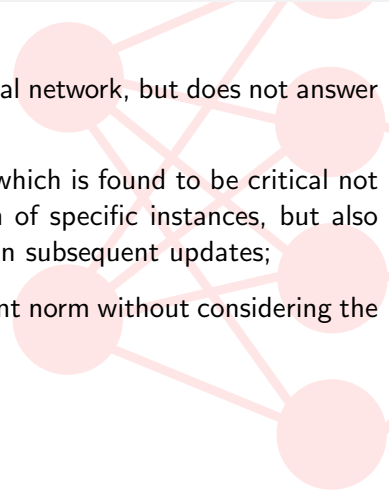
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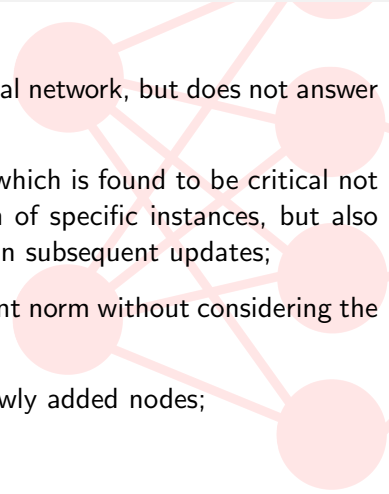
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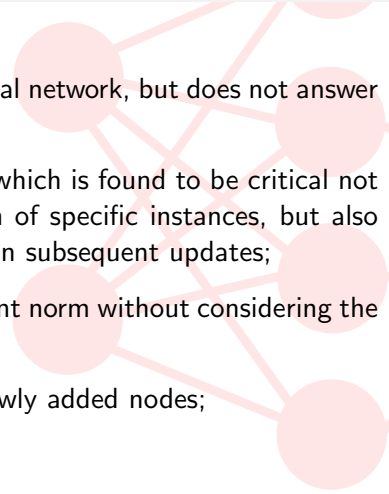
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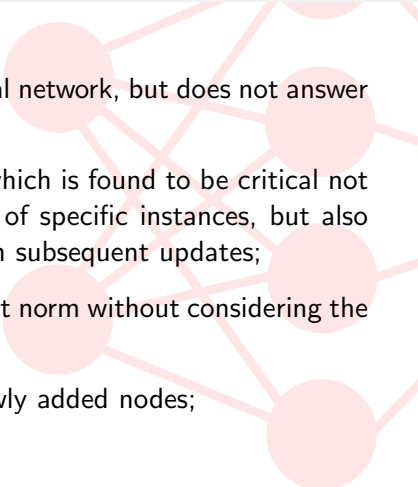
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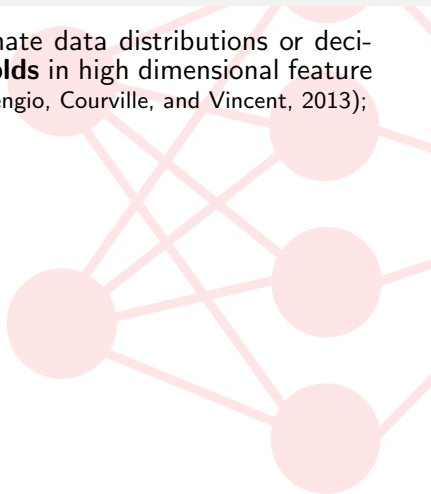
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Preliminaries - The Manifold Hypothesis

- DNNs can be seen as to approximate data distributions or decision boundaries by learning **manifolds** in high dimensional feature spaces (Bengio, Mesnil, et al., 2013; Bengio, Courville, and Vincent, 2013);



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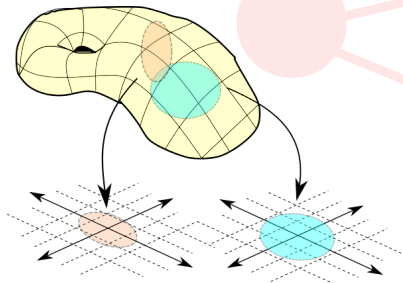
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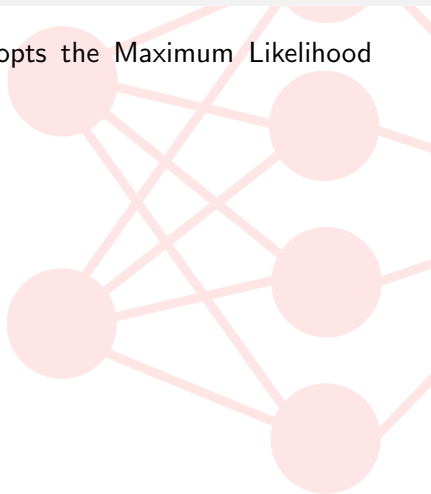
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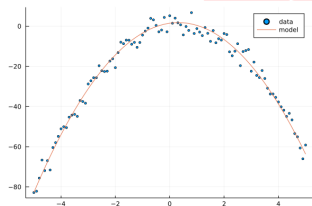
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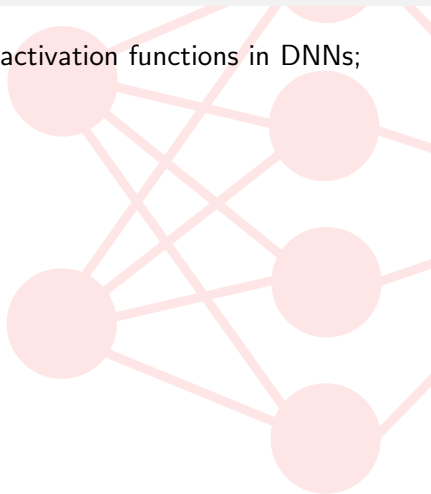
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deep ReLU networks are equivalently replicable by corresponding shallow ReLU networks with only one hidden layer.

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Deep ReLU Networks Have Surprisingly Few Activation Patterns

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Abstract

The number of deep networks has been estimated to grow to such an extent that it is impossible to even approximate the number of possible activation patterns. In this paper, we show that the number of activation patterns is actually quite small. We show that the number of activation patterns is bounded by the number of neurons in the input layer. We show that the number of activation patterns is bounded by the number of neurons in the input layer. We show that the number of activation patterns is bounded by the number of neurons in the input layer.

1 Introduction

A fundamental question in the theory of deep learning is why shallow networks often work as well as deep networks. One proposed explanation is that shallow networks are more expressive than deep networks. This paper provides evidence for this claim by showing that the number of activation patterns in deep networks is actually quite small.

In this note, we attempt to answer the question: how many activation patterns are possible in a deep network? We show that the number of activation patterns is bounded by the number of neurons in the input layer. We show that the number of activation patterns is bounded by the number of neurons in the input layer.

We present our results in the form of a theorem. This theorem has been the subject of previous work (e.g., Rolnick et al., 2018; Hanin et al., 2020). Our results are based on a new proof technique that we call “XNG by Folding”.

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DEEP EQUALS SHALLOW FOR RELU NETWORKS IN KERNEL REGIMES

Alejo José G. Sison
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David Rolnick
University of Toronto
rolnick@cs.toronto.edu

ABSTRACT

Deep networks are often considered to be more expressive than shallow ones. In this paper, we show that this is not the case. We show that the number of activation patterns in deep networks is actually quite small. We show that the number of activation patterns in deep networks is actually quite small. We show that the number of activation patterns in deep networks is actually quite small.

1 INTRODUCTION

The question of which functions can be well approximated by neural networks is central to understanding why these models are so successful. One proposed explanation is that shallow networks are more expressive than deep networks. This paper provides evidence for this claim by showing that the number of activation patterns in deep networks is actually quite small.

We present our results in the form of a theorem. This theorem has been the subject of previous work (e.g., Rolnick et al., 2018; Hanin et al., 2020). Our results are based on a new proof technique that we call “XNG by Folding”.



Rates of approximation by ReLU shallow neural networks

Teng Ma¹, Qing Xiao²

¹Department of Mathematics, University of Toronto, Toronto, Canada
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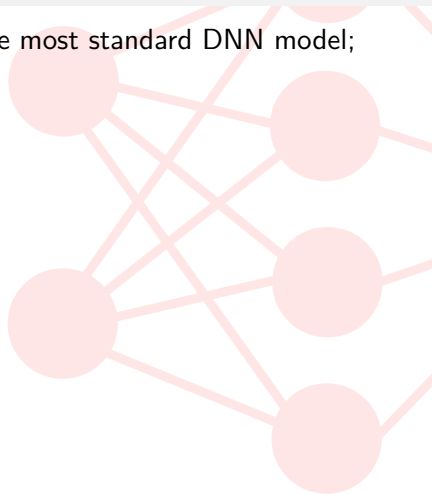
ABSTRACT

Neural networks activated by the rectified linear unit (ReLU) are a central topic in the theory of approximation. In this paper, we study the rates of approximation by shallow ReLU networks. We show that the number of activation patterns in deep networks is actually quite small. We show that the number of activation patterns in deep networks is actually quite small. We show that the number of activation patterns in deep networks is actually quite small.

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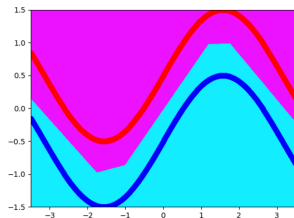
The manifolds approximated by ReLU-based MLP models are locally linear, consisting of multiple linear hyper-planes. Each linear segment corresponds to a different activation pattern of the ReLU units, giving the model its ability to approximate a locally linear behavior within each segment.

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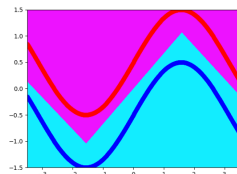
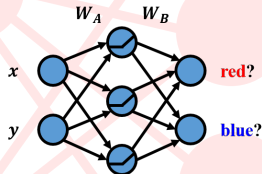
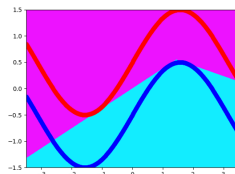
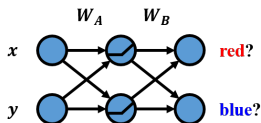
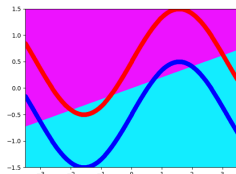
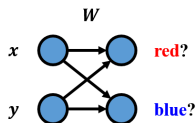


Preliminaries - Growing DNNs Increase Non-linearity

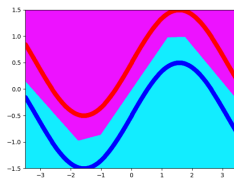
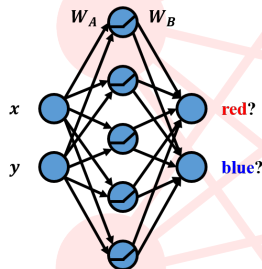
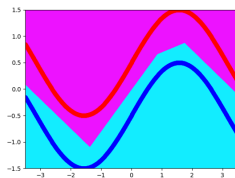
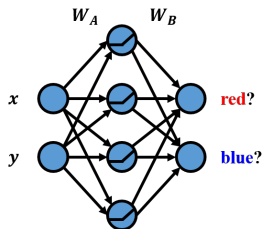
Observation 1

Growing a DNN by adding new node(s) to broaden a specific layer introduces new dimension(s) to the latent feature space associated with that layer, which is, in nature, increasing the non-linearity of the low-dimensional projections of the manifold to enhances the network's capacity to model complex patterns.

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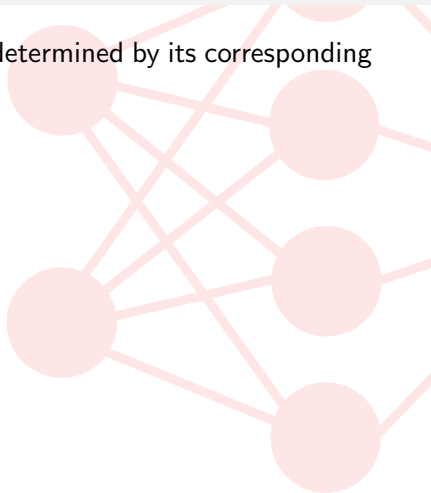


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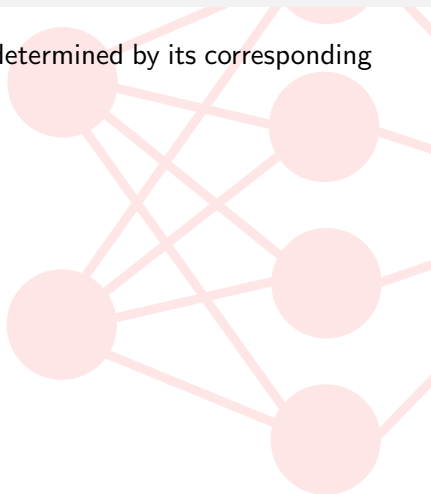
Key Ideas

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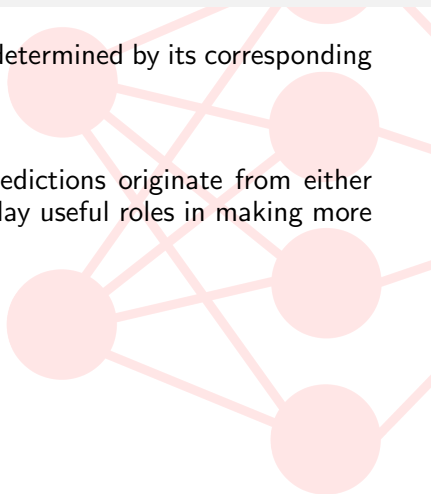
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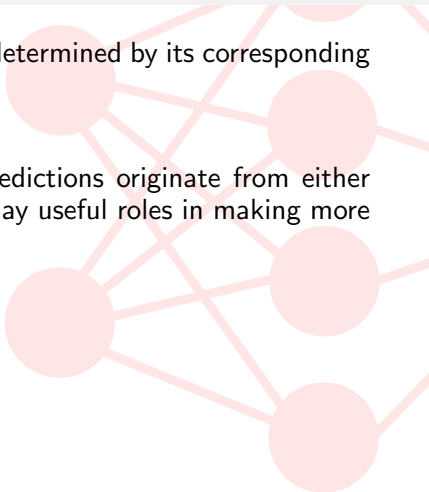
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- ④ Specifically, the model's capability (i.e., approximatability) can be increased by introducing non-linearity to its complexity,
- ⑤ which, can be achieved by breaking / folding the corresponding activated linear segment that leads to the typical mis-prediction.

Definitions

Definition (Activated Linear Segment)

For manifolds in high-dimensional spaces that are approximated by ReLU-based MLPs, their projections onto the input space are locally linear. In classification tasks, these projections are the decision boundaries, whereas in prediction tasks, they are the regression curves. Each piece of linear segments of these projections results from a composition of affine transformations governed by a specific activation pattern of ReLU units. These segments can thus be called "activated linear segments".

Definitions

Definition (Decision Boundary)

An $n - 1$ dimensional hyper-plane on the n dimensional input space for distinguishing between two classes (the wrongly predicted class i given input and its ground truth class j), which is defined by equation $\mathbf{w}_{i-j}^{\vec{}} \cdot \vec{\mathbf{x}} + b_{i-j} = 0$, where $\mathbf{w}_{i-j}^{\vec{}}$ and b_{i-j} denote the differences between row i and row j of the affine transformation of the corresponding activated linear segment.

Definitions

Definition (Folding Crease)

An $n - 2$ dimensional sub-space on the $n - 1$ dimensional hyper-plane of the decision boundary that acts as the "transition line" between two contiguous activated linear segments, where the activation pattern changes.

Definition (Fold Point)

A single point \vec{x}_f (an n dimensional vector) on the Folding Crease that can use for guiding the location of Folding Crease on the $n - 1$ dimensional hyper-plane of the decision boundary:

$$\begin{cases} \vec{w}_{i-j} \cdot \vec{x} + b_{i-j} = 0 \\ \vec{u} \cdot (\vec{x} - \vec{x}_f) = 0 \end{cases} \quad \text{where } \vec{u} \text{ is a non-zero } n \text{ dimensional vector}$$

that is orthogonal to the normal vector of the $n - 1$ dimensional hyper-plane of the decision boundary \vec{w}_{i-j} , i.e. $\vec{u} \cdot \vec{w}_{i-j} = 0$

Definitions

Definition (Typical Mis-predicted Instance)

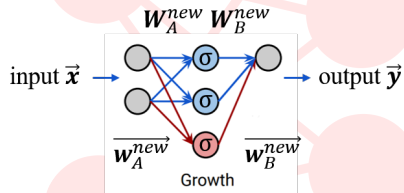
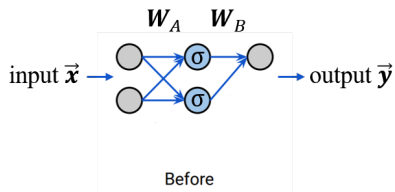
Among all input data that is wrongly predicted by an model, the single input data instance that can be represents a certain kind of mistakes that the model cannot distinguish is called a "typical mis-predicted instance".

Determining Values for New Parameters

Theorem 3

Adding a Folding Crease on the Decision Boundary of an existing Activated Linear Segment at a specific location \vec{x}_f can be implemented by introducing a new node to the first layer of the shallow ReLU network and enforce the activation of its parameters (denoted as \vec{w}_A^{new} and b_A^{new} respectively) to occur exactly at point \vec{x}_f using the equation $\vec{w}_A^{new} \cdot \vec{x}_f + b_A^{new} = 0$.

Notations & Symbols



$$W_A^{new} = \begin{bmatrix} W_A \\ \overrightarrow{w_A^{new}} \end{bmatrix}$$

$$W_B^{new} = \begin{bmatrix} W_B & \overrightarrow{w_B^{new}} \end{bmatrix}$$

Determining Values for New Parameters

Lamma 1

If and only if the $\mathbf{w}_A^{\vec{n}^{new}}$ can be represented as an linear combination of $\mathbf{w}_{i-j}^{\vec{n}}$ and \vec{u} (i.e. there exist scalars α and β such that $\mathbf{w}_A^{\vec{n}^{new}} = \alpha \mathbf{w}_{i-j}^{\vec{n}} + \beta \vec{u}$), there is one and only one solution for variable b_A^{new} that for all input \vec{x} on the Folding Crease, satisfy the above equation $\mathbf{w}_A^{\vec{n}^{new}} \cdot \vec{x} + b_A^{new} = 0$.

Determining Values for New Parameters

Lamma 2

$$\frac{d\mathcal{L}}{d\vec{x}} = (\mathbf{W}_B \sigma(\cdot)' \mathbf{W}_A)^T \frac{d\mathcal{L}}{d\vec{y}} + (\mathbf{w}_B^{\vec{new}} \cdot \frac{d\mathcal{L}}{d\vec{y}}) \mathbf{w}_A^{\vec{new}}$$

Theorem 4

$\mathbf{w}_A^{\vec{new}}$ directly affect the direction of $\frac{d\mathcal{L}}{d\vec{x}}$ by specifying the direction of its component vector, while $\mathbf{w}_B^{\vec{new}}$ indirectly affect $\frac{d\mathcal{L}}{d\vec{x}}$ by determining the norm of its component vector.

Determining Values for New Parameters

Lamma 3

$\mathbf{w}_A^{\vec{n}^{ew}}$ directly determines which input domains can activate the newly added node

Theorem 5

$\mathbf{w}_A^{\vec{n}^{ew}}$ determines the location of the fold point after adding a new node.

Determining Values for New Parameters

Lamma 4

To ensure the affine transformation of the Activated Linear Segment does not vary much before and after introducing the new node, the parameters of the newly added connection in the second layer of the network model (denoted as $\mathbf{w}_B^{\vec{n}ew}$) need to approach:

$$\left\{ \begin{array}{l} \mathbf{w}_A^{\vec{n}ew} \otimes \mathbf{w}_B^{\vec{n}ew} \rightarrow \mathbf{0}_{n,n} \\ b_A^{new} \cdot \mathbf{w}_B^{\vec{n}ew} \rightarrow \vec{0} \end{array} \right. \quad \text{which can be further simplified}$$

$$\text{as: } \min \|\mathbf{w}_B^{new}\|^2$$

Lamma 5

The above $\|\mathbf{w}_B^{new}\|^2$ cannot be exactly equal to zero, otherwise no gradient can be backpropagated to update the corresponding parameters $\mathbf{w}_A^{\vec{n}ew}$ and b_A^{new} in the first layer.

Proposed Method

Algorithm: Grow by Folding

initialize training dataset $\mathbb{X} = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$, where $\mathbf{x}_i \sim \mathbb{D}$ ($i \in \{1, 2, \dots, n\}$, \mathbb{D} is the input space)

initialize shallow ReLU MLP model f with parameters $\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B$

do loop: train f on \mathbb{X} until converge

find the most typical mis-predicted instance and a fold point on the decision boundary:

$\mathbf{x}_t, \mathbf{x}_f = \text{fold_point_search}(\mathbb{X}, f)$, where $\mathbf{x}_f \sim \mathbb{D}$

calculate new parameters for the broaden model:

$\mathbf{W}_A^{new}, \mathbf{b}_A^{new}, \mathbf{W}_B^{new} = \text{hidden_layer_broaden}(\mathbf{x}_t, \mathbf{x}_f, f)$

create new model and apply new parameters as initial values:

$f_{\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B} \leftarrow f_{\mathbf{W}_A^{new}, \mathbf{b}_A^{new}, \mathbf{W}_B^{new}, \mathbf{b}_B}$

$f_{\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B} \leftarrow \text{equivalent_network_deepening}(f_{\mathbf{W}_A, \mathbf{b}_A, \mathbf{W}_B, \mathbf{b}_B})$

Proposed Method

Algorithm: Fold Point Search

input training dataset \mathbb{X}

input shallow ReLU MLP model f with parameters W_A, b_A, W_B, b_B

find the most typical mis-predicted instance:

$$\mathbf{x}_t = \text{find_typical_mis_predicted_instance}(\mathbb{X}, f)$$

find the activated linear segment of model f given \mathbf{x}_t as input:

$$W_{\text{activated}}, b_{\text{activated}} = \text{find_activate_linear_segment}(\mathbf{x}_t, W_A, b_A, W_B, b_B)$$

decision boundary regarding \mathbf{x}_t can be defined by:

$$\{\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_\infty\} \text{ s.t. } W_{\text{activated}}\mathbf{x}_i + b_{\text{activated}} = \mathbf{c}, \text{ where } \mathbf{c} \text{ is a uniform vector}$$

find the fold point \mathbf{x}_f on the decision boundary that is closest to \mathbf{x}_t :

$$\mathbf{x}_f = \min_{d \in \{\mathbf{d}_1, \mathbf{d}_2, \dots, \mathbf{d}_\infty\}} \|\mathbf{d} - \mathbf{x}_t\|^2$$

output $\mathbf{x}_t, \mathbf{x}_f$

Proposed Method

Algorithm: Find Typical Mis-Predicted Instance

input training dataset \mathbb{X}

input shallow ReLU MLP model f with parameters W_A, b_A, W_B, b_B

sample subset $\mathbb{S} = \{\mathbf{x}_a, \mathbf{x}_b, \dots, \mathbf{x}_m\}$ from \mathbb{X}

feed \mathbb{S} into the model f and calculate their corresponding **values of loss function** $\mathbb{L} = \{l_a, l_b, \dots, l_m\}$

performing **weighted k-means clustering** on \mathbb{S} using corresponding \mathbb{L} as weights and get clusters $\{\mathbb{C}_1, \mathbb{C}_2, \dots, \mathbb{C}_k\}$

calculate average loss for instances in each clusters $\{l_{\mathbb{C}_1}, l_{\mathbb{C}_2}, \dots, l_{\mathbb{C}_k}\}$

find the cluster \mathbb{C}_i that has the highest average loss $l_i = \max(\{l_{\mathbb{C}_1}, l_{\mathbb{C}_2}, \dots, l_{\mathbb{C}_k}\})$

find instance $\mathbf{x}_t = \min_{\mathbf{x}_i \in \mathbb{C}_i} \|\mathbf{x}_i - \mathbf{x}_c\|^2$, where \mathbf{x}_c is the centroid of \mathbb{C}_i

output \mathbf{x}_t

Proposed Method

Algorithm: Hidden Layer Broaden

input typical mis-predicted point x_t

input fold point on the decision boundary x_f

input shallow ReLU MLP model f_{W_A, b_A, W_B, b_B} with parameters W_A, b_A, W_B, b_B

ensure $\forall x: W_B^{new} W_A^{new} x = W_B W_A x$:

set $W_B^{new} = [W_B \quad \mathbf{0}]$

set $b_A^{new} = \begin{bmatrix} b_A \\ 0 \end{bmatrix}$

set $W_A^{new} = \begin{bmatrix} W_A \\ W_A^+ \end{bmatrix}$ s.t.:

ensure the grown new model fold only at point x_f :

$$W_A^{new} x_f + b_A^{new} = \mathbf{0}$$

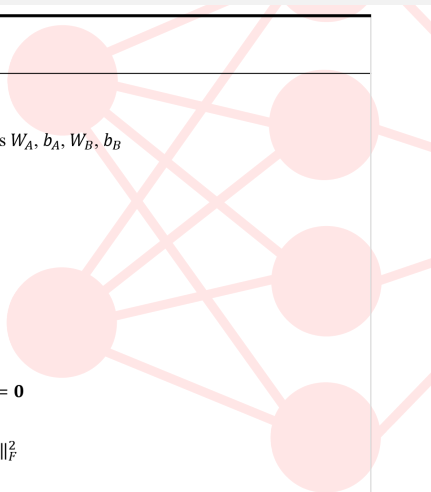
apply GradMax to W_A^{new}

$$\max_{W_A^{new}} \|\mathbb{E}_{\mathbb{D}} \nabla W_A^{new}\|_F^2$$

align gradient direction with $W_A^{new}(x_t - x_f)$

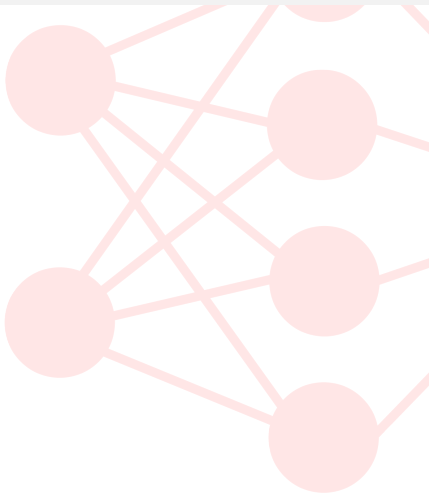
$$\max_{W_A^{new}} \frac{\nabla W_A^{new} x_t \cdot W_A^{new}(x_t - x_f)}{\|\nabla W_A^{new} x_t\| \cdot \|W_A^{new}(x_t - x_f)\|}$$

output $W_A^{new}, b_A^{new}, W_B^{new}$



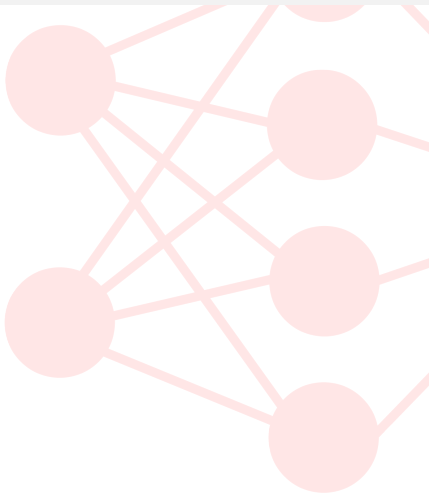
Supplementary Details

1 "Dead Layer" Problem



Supplementary Details

- 1 "Dead Layer" Problem
 - Batch Normalization



Supplementary Details

- ① "Dead Layer" Problem
 - Batch Normalization
- ② Optimization Problem of Fold Point Search Algorithm



Supplementary Details

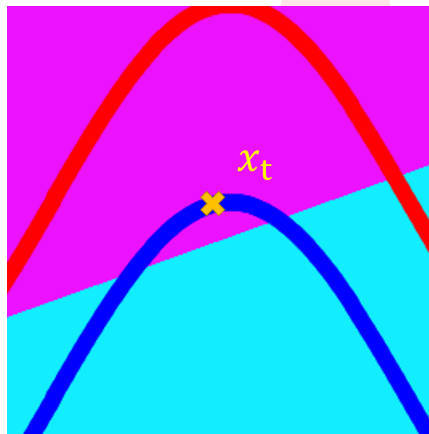
① "Dead Layer" Problem

- Batch Normalization

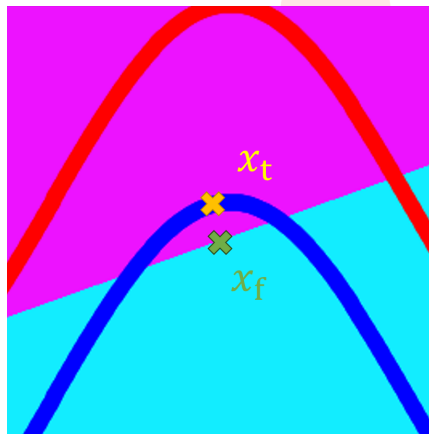
② Optimization Problem of Fold Point Search Algorithm

- given the equation of decision boundary: $w \cdot x + b = 0$, the closest point on the decision boundary can be found by
$$x_t - ((w \cdot x_t) + b) * (w / (w \cdot w))$$

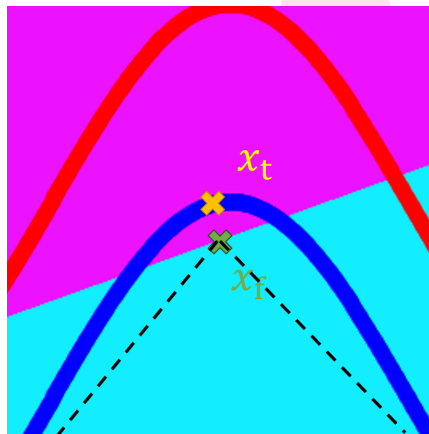
Example



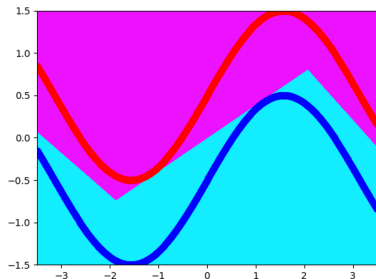
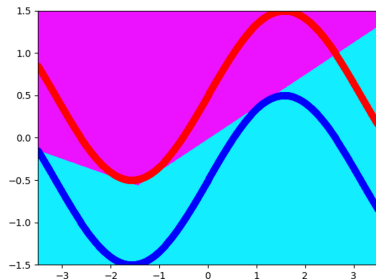
Example



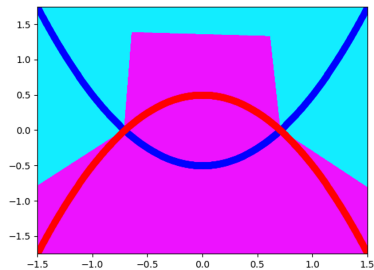
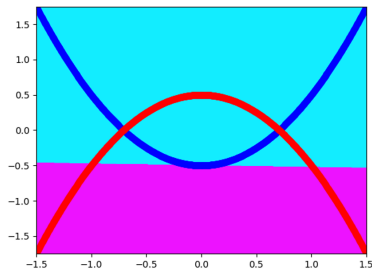
Example



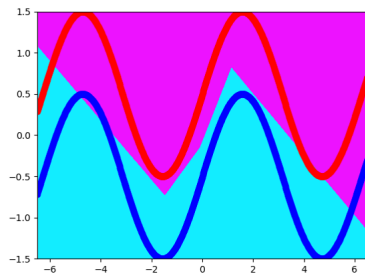
Binary Classification: Sine



Binary Classification: Overlap Quadratic



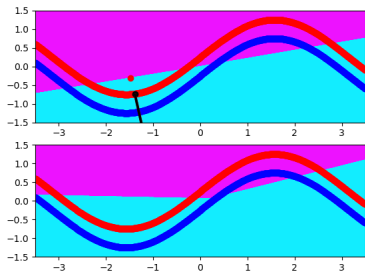
Utilization of Approximatability



- random initialized: **65** / 1000
- grow from 2-2-2 to 2-3-2: **360** / 1000

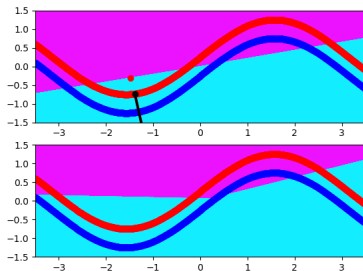
Next Milestones

- 1 due to the difference in updating speeds between the old and new parameters, the proposed direction along $\vec{x}_t - \vec{x}_f$ is not the most ideal gradient direction for updates



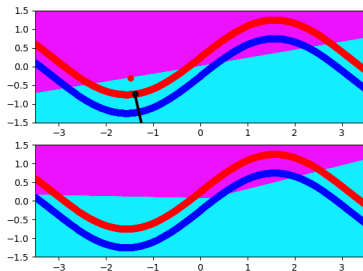
Next Milestones

- ① due to the difference in updating speeds between the old and new parameters, the proposed direction along $\vec{x}_t - \vec{x}_f$ is not the most ideal gradient direction for updates
- ② Folding point does not lie on the effective activated linear segment



Next Milestones

- 1 due to the difference in updating speeds between the old and new parameters, the proposed direction along $\vec{x}_t - \vec{x}_f$ is not the most ideal gradient direction for updates
- 2 Folding point does not lie on the effective activated linear segment
- 3 Constrained Optimization Difficulty



References I

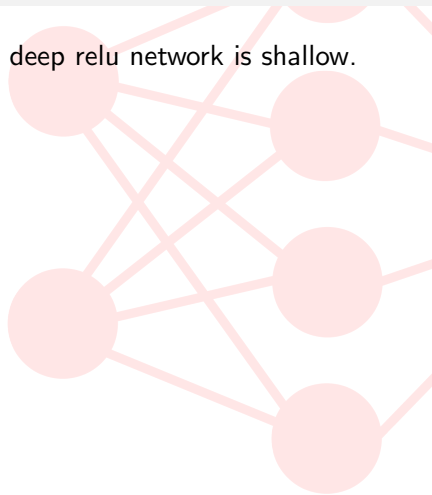
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Thank you!

